Investigation

Description

The ISA-TAB-Nano investigation file leverages the ISA-TAB investigation file, and it allows for the description of the primary investigation and associated studies including assays and protocols. An investigation can have one or more studies. For example, an investigation titled "Dendrimer-Based MRI Contrast Agents" may have two studies titled as "Characterizing the Size of Dendrimer based MRI Contrast Agents" and "Determining the cytotoxicity property of Dendrimer based MRI Contrast Agents in porcine proximal tubule cells" Each study can have one or more assays depending on the endpoint measured and the technique used. For example, a cytoxicity study may be conducted using an MTT assay and a LDH release assay. While a size characterization study can include two types of assays based on the technique used – one using DLS and the other using AFM.

The ISA-TAB specification provides flexibility in representing the level of granularity in information associated with a study; however, the level of granularity should factor in the effective representation of assays and protocols in conformance with the specification. For example, a study focusing on "Size Characterizations" will have multiple size measurements (for example, Z-average size, hydrodynamic size) and may involve the use of multiple techniques (for example, size by DLS, size by AFM). These can be represented effectively in the ISA-TAB file structure that ISA-TAB-Nano uses.

The investigation file provides descriptive information about studies including design descriptors, publications, factors, assays, protocols, and contacts. This descriptive information lays the foundation for other ISA-TAB-Nano files. For example, TABLE 1 shows a subset of the Investigation File, which is the study factors section of the investigation file. This section provides the names of factors (for example, temperature, solvent medium) used in the study and their associated units of measurement (if the factors are quantitative). The values of these factors (for example, PBS, 25 Celsius) are specified either in the study or the assay file.

File Format

The ISA-TAB-Nano investigation file leverages the ISA-TAB file format, which is a vertical-based spreadsheet format with row headers in the first column, as shown in TABLE 1. The fields are divided into sections. Therefore, the field values in the investigation file are entered in column order. For instance, in TABLE 1, Column A indicates the field names and Columns B and C contain the field values.

TABLE 1 Example Subset of the Investigation File Format

A	B	C
STUDY FACTORS	N/A	N/A
Study Factor Name	temperature	solvent
Study Factor Type	temperature	solvent medium
Study Factor Type Term Accession Number	PATO_0000146	NPO_1855

Study Factor Type Term Source REF	PATO	NPO

Fields

The field names in an investigation file are organized vertically in the first column. These fields are divided into 11 sections as defined by ISA-TAB. These sections are:

- ONTOLOGY SOURCE REFERENCE
- INVESTIGATION
- INVESTIGATION PUBLICATIONS
- INVESTIGATION CONTACTS
- MATERIAL
- STUDY
  - STUDY DESIGN DESCRIPTORS
  - STUDY PUBLICATIONS
  - STUDY FACTORS
  - STUDY ASSAYS
  - STUDY PROTOCOLS
  - STUDY CONTACTS

ISA-TAB-Nano Extensions--- ISA-TAB-Nano extends the ISA-TAB Investigation File specification by introducing new fields. All fields are defined below.

Ontology Source Reference

This section is used to record information about ontologies containing the terms referenced in the ISA-TAB-Nano files. TABLE 1 on the Investigation File Example page shows an example of the ONTOLOGY SOURCE REFERENCE section along with example data. This section uses four ISA-TAB concepts:

Term Source Name---The name of the source from where a term is selected and referenced in the ISA-TAB-Nano files. The source could be an ontology or a controlled vocabulary. The source name is the full name or the acronym of the ontology/controlled vocabulary. This is a required field if the term source name is referenced in any of the ISA-TAB-Nano files.

T erm Source File--- A file name or a URI of the source named in the *term source name* field.

Term Source Version---Version number of the vocabulary source file. This is a required field if the field for *term source file* has a value.

Term Source Description---Text description to disambiguate resources when homologous acronyms are used.

Investigation

This section allows for the description of the investigation. An example of the INVESTIGATION section is in TABLE 2 on the Investigation File Example page. The INVESTIGATION section uses nine concepts and includes concepts from ISA-TAB and extensions made in support of ISA-TAB-Nano:

Investigation Identifier--- A locally unique identifier or an accession number provided by a repository.

Investigation Title---A concise phrase used as a title for the investigation.

Investigation Description---A textual description of the investigation.

Investigation Dubmission Date---The date on which the investigation was reported to a repository (format: YYYY-MM-DD).

Investigation Public Release Date---The date on which the investigation is publicly released or published (format: YYYY-MM-DD).

Investigation Disease---Disease(s) that are the subject of an investigation, if applicable. This concept is introduced in ISA-TAB-Nano to identify the disease(s) related to the subject of the investigation. (ISA-TAB Extension for ISA-TAB-Nano)

Investigation Disease Term Accession Number---Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *investigation disease*. This concept is introduced in ISA-TAB-Nano to identify the term accession number for the disease. (ISA-TAB Extension for ISA-TAB-Nano)

Investigation Disease Term Source REF--- The name which identifies the source from where the term for *investigation disease* is selected. This name should match one of the names entered in the *term source name* field. This concept is introduced in ISA-TAB-Nano to identify the term source ref for the disease. (ISA-TAB Extension for ISA-TAB-Nano)

Investigation Outcome---A textual description summarizing the conclusion of an investigation. This concept is introduced in ISA-TAB-Nano to identify the outcome of the investigation. (ISA-TAB Extension for ISA-TAB-Nano)

Investigation Publications

This section allows for the identification of articles (published) associated with the investigation. An example of the INVESTIGATION PUBLICATIONS section is in TABLE 3 on the Investigation File Example page. There are seven ISA-TAB concepts used in this section:

Investigation Pubmed ID---PubMed identifier of the publication associated with the investigation.

Investigation Publication DOI---A Digital Object Identifier (DOI) of the publication associated with the investigation.

Investigation Publication Author List---A semicolon-delimited (";") list of authors of a publication associated with the investigation.

Investigation Publication Title---A concise phrase used as a title for the publication associated with the investigation.

Investigation Publication Status---A term describing the status of a publication (that is, submitted, in preparation, published).

Investigation Publication Status Term Accession Number---The identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *investigation publication status*.

Investigation Publication Status Term Source REF---The name which identifies the source from where the term for *investigation publication status* is selected. This name should match one of the names entered in the *term source name* field.

Investigation Contacts

This section allows for the identification of the point(s) of contact for the investigation. An example of the INVESTIGATION CONTACTS section is in TABLE 4 on the Investigation File Example page. There are 11 ISA-TAB concepts used as field names: An example of the INVESTIGATION CONTACTS section is in TABLE 4 on the Investigation File Example page. There are 11 ISA-TAB concepts used as field names:

Investigation Person Last Name---The last name of a person who is the point of contact for the investigation.

Investigation Person First Name---The first name of a person who is the point of contact for the investigation.

Investigation Person Mid Initials---The middle initial(s) of a person who is the point of contact for the investigation.

Investigation Person Email---The email address of a person who is the point of contact for the investigation.

Investigation Person Phone---The telephone number of a person who is the point of contact for the investigation.

Investigation Person Fax---The fax number of a person who is the point of contact for the investigation.

Investigation Person Address---The mailing address of a person who is the point of contact for the investigation.

Investigation Person Affiliation--- The name of the organization to which the point of contact belongs.

Investigation Person Roles--- The term which classifies the role(s) performed by person who is the point of contact for the investigation.

Investigation Person Roles Term Accession Number--- Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *investigation person role*.

Investigation Person Roles Term Source REF--- Name of the ontology or controlled vocabulary from which a term is selected and entered as a value for *investigation person role*.

Material

This section allows for the identification of materials used in the investigation and associated studies. There are 2 concepts used in the MATERIAL section. An example of the MATERIAL section is in TABLE 5 on the Investigation File Example page. The MATERIAL section is introduced in ISA-TAB-Nano. These concepts are described below:

Material File Name---The name of the ISA-TAB-Nano Material File, which lists information about the composition and characteristics of the nanomaterials or other small molecules. There can be only one file per cell. This concept is introduced in ISA-TAB-Nano to identify the name of the Material File. (ISA-TAB Extension for ISA-TAB-Nano)

Material Source Name---The name of the nanomaterial or small molecule associated with the Material File. There can be only one Material Source Name per column. This concept is introduced in ISA-TAB-Nano to identify source name of the material. (ISA-TAB Extension for ISA-TAB-Nano)

Study

This section allows for the description of one or more studies conducted as part of an investigation. An example of the STUDY section is in TABLE 6 on the Investigation File Example page. There are 11 concepts used in the STUDY section, seven of which are taken from ISA-TAB and four are introduced in ISA-TAB-Nano. These concepts are described below:

Study Identifier---A unique identifier used for the study. It is either a temporary identifier supplied by users or one generated by a repository or

other database.

Study Title---A concise phrase used to encapsulate the purpose and goal of the study.

Study Description---A textual description of the study, with components such as objectives or goals.

Study Submission Date---The date on which the study is submitted to an archive (format: YYYY-MM-DD).

Study Public Release Date---The date on which the study is publicly released or published (format: YYYY-MM-DD).

Study Disease---Disease(s) that are the subject of the study, if applicable. This concept is introduced in ISA-TAB-Nano to identify the disease(s) related to the study. (ISA-TAB Extension for ISA-TAB-Nano)

Study Disease Term Accession Number---Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *study disease*. (ISA-TAB Extension for ISA-TAB-Nano)

Study Disease Term Source REF---The name which identifies the source from where the term for *study disease* is selected. This name should match one of the names entered in the *term source name* field. (ISA-TAB Extension for ISA-TAB-Nano)

Study Outcome---A textual description about the outcome(s) of the study. This concept is introduced in ISA-TAB-Nano to provide a summary or conclusion of a study. (ISA-TAB Extension for ISA-TAB-Nano)

Study File Name---The name of the ISA-TAB-Nano study file, which lists information about the biological specimens (cells, tissues, organs, animal model, body fluids), nanoparticles; small organic molecules, and other types of samples assayed in a study. There can be only one file name per cell.

Study Design Descriptors

This section allows for the identification of design type of the study. An example of the STUDY DESIGN DESCRIPTORS section is in TABLE 7 on the Investigation File Example page. There are 3 concepts used in the STUDY DESCRIPTORS section. These concepts are taken from ISA-TAB.

Study Design Type---A term describing the classification of the study based on the overall study (experimental) design (for example, comparison study). The term can be free-text or taken from a controlled vocabulary/ontology.

Study Design Type Term Accession Number---Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *study design type.*

Study Design Type Term Source REF---The name which identifies the source from where the term for *study design type* is selected. This name should match one of the names entered in the *term source name* field.

Study Publications

This section allows for the identification of articles (published) associated with the study. An example of the STUDY PUBLICATIONS section is in TABLE 8 on the Investigation File Example page. . This section uses seven ISA-TAB concepts.

Study Pubmed ID---PubMed identifier of the publication associated with the study.

Study Publication DOI---A Digital Object Identifier (DOI) of the publication associated with the study.

Study Publication Author List---A semicolon-delimited (";") list of authors of a publication associated with the study.

Study Publication Title---A concise phrase used as a title for the publication associated with the study.

Study Publication Status---A term describing the status of a publication (that is, submitted, in preparation, published), associated with the study.

Study Publication Status Term Accession Number---The identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *study publication status.*

Study Publication Status Term Source REF---The name which identifies the source from where the term for *study publications status* is selected. This name should match one of the names entered in the *term source name.*

Study Factors

This section allows for the identification of factors associated with the study. An example of the STUDY FACTORS section is in TABLE 9 on the Investigation File Example page. This section has four concepts taken from ISA-TAB.

Study Factor Name---The name of one independent variable (factor) manipulated by the experimentalist with the intention to affect the subject of study (that is, Stressor). This is a required field, if there are factors in an assay study. Only one factor name is allowed per cell. The value of a factor is given either in the study or in the assay file.

Study Factor Type---A term used for the classification of factors associated with the study (for example, condition). This is a required field if there are factors in an assay study. More than one term is allowed per cell; multiple terms are separated by semicolons.

Study Factor Type Term Accession Number---Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *study factor type*.

Study Factor Type Term Source REF---The name which identifies the source from where the term for *study factor type* is selected. This name should match one of the names entered in the *term source name* field.

Study Assays

This section allows for the identification of type of measurement and the type of technology used for the measurement in an assay that is part of a study. An example of the STUDY ASSAYS section is in TABLE 10 on the Investigation File Example page. The STUDY ASSAYS section has 11 concepts. Out of these, 8 concepts are taken from ISA-TAB. The remaining concepts are introduced in ISA-TAB-Nano.

Study Assay Measurement Type---A term to qualify the endpoint, or what is being measured.

Study Assay Measurement Type Term Accession Number---Identification number of the term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *study assay measurement type*.

Study Assay Measurement Type Term Source REF---The name which identifies the source from where the term for *study assay measurement type* is selected. This name should match one of the names entered in the *term source name* field.

Study Assay Technology Type---The type of technology (technique or method) used for the assay measurement (for example, Dynamic light scattering).

Study Assay Technology Type Term Accession Number---Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *study assay technology type*.

Study Assay Technology Type Term Source REF---The name which identifies the source from where the term for *study assay technology type* is selected. This name should match one of the names entered in the *term source name* field.

Study Technology Platform---The manufacturer and platform name of the instruments used in the study assay.

Study Assay Measurement Name---A semicolon-delimited list of names of quantities whose values are the outputs of an assay measurement. (ISA-TAB Extension for ISA-TAB-Nano)

Study Assay Measurement Name Term Accession Number---Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *study assay measurement name*. (ISA-TAB Extension for ISA-TAB-Nano)

Study Assay Measurement Name Term Source REF--- The name which identifies the source from where the term for *study assay measurement name* is selected. (ISA-TAB Extension for ISA-TAB-Nano)

Study Assay File Name--- Name of the ISA-TAB-Nano Assay file corresponding to the study assay. This is a required field. There can be only one assay file name per cell.

Study Protocols

This section allows for the identification of the type of protocols, and the parameters and components of a protocol used in a study. A protocol describes the formal plan of an experiment or research activity, including the objective, rationale, design, materials and methods for the conduct of the study; intervention description, and method of data analysis. An example of the STUDY PROTOCOLS section is in TABLE 11 on the Investigation File Example page. There are 14 concepts in this section taken from ISA-TAB.

Study Protocol Name---The name of the protocols used within a study and will be referenced in the ISA-TAB-Nano Study or Assay files.

Study Protocol Type---The term used to classify the protocol (for example, synthesis, assay, etc.).

Study Protocol Type Term Accession Number--- Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *study protocol type*

Study Protocol Type Term Source REF---Name of the ontology or controlled vocabulary from which a term is selected and entered as a value for *study protocol type*.

Study Protocol Description---A textual description of the protocol.

Study Protocol URI---Pointer to protocol documents or resources external to ISA-TAB-Nano, which can be accessed by their Uniform Resource Identifier (URI). If URI is not available, enter the protocol document file name and make the protocol document available along with ISA-TAB-Nano files.

Study Protocol Version---An identifier for the version to ensure protocol tracking.

Study Protocol Parameters Name---A semicolon-delimited (";") list of parameter names used as an identifier in the ISA-TAB-Nano Study or Assay files. A protocol parameter is a constant associated with a protocol, which is not varied as part of an experiment.

Study Protocol Parameters Name Term Accession Number---Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for the *study protocol parameter name*.

Study Protocol Parameters Name Term Source REF---The name which identifies the source from where the term for *study protocol parameter name*. This name should match one of the names entered in the *term source name* field.

Study Protocol Components Name--- A semicolon-delimited (";") list of names identifying the components of a protocol. Component names include instrument names, software names, and reagent names.

Study Protocol Components Type--- The term to classify the protocol component, for example, instrument, software, and reagent.

Study Protocol Components Type Term Accession Number--- Identification number of a term seleced from an ontology or a controlled vocabulary, if the term is entered as a value for the *study protocol component type*.

Study Protocol Components Type Term Source REF--- The name which identifies the source from where the term for *study protocol component type* is selected. This name should match one of the names entered in the *term source name* field.

Study Contacts

This section allows the identification of the point of contact for a study. An example of the STUDY CONTACTS section is in TABLE 12 on the Investigation File Example page. The STUDY CONTACTS section has 11 ISA-TAB concepts.

Study Person Last Name---The last name of a person who is the point of contact for the study.

Study Person First Name---The first name of a person who is the point of contact for the study.

Study Person Mid Initials---The middle initial(s) of a person who is the point of contact for the study.

Study Person Email---The email address of a person who is the point of contact for the study.

Study Person Phone---The telephone number of a person who is the point of contact for the study.

Study Person Fax--- The fax number of a person who is the point of contact for the study

Study Person address--- The mailing number of a person who is the point of contact for the study

Study Person Affiliation--- The name of the organization to which the point of contact belongs.

Study Person Roles--- The term which classifies the role(s) performed by person who is the point of contact for the study.

Study Person Roles Term Accession Number--- Identification number of a term selected from an ontology or a controlled vocabulary, if the term is entered as a value for *study person role*.

Study Person Roles Term Source REF--- The name which identifies the source from where the term for *study person role* is selected. This name should match one of the names entered in the *term source name* field.

Files

The Investigation File Examples, Template, and Glossary are listed here.

- Investigation File Example
- Investigation File Template
- Investigation File Glossary

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